Theoretical Solid State Physics and Statistical Mechanics Group I(Annual Report)

journal or publication title	The science reports of the Tohoku University. Ser. 8, Physics and astronomy
volume	10
number	1
page range	35-41
year	1989-07-25
URL	http://hdl.handle.net/10097/25680

Theoretical Solid State Physics and Statistical Mechanics Group I

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ResearchActivities

(I)HIGH-ENERGY SPECTROSCOPY IN *f* AND *d* ELECTRON SYSTEMS

a. Many-Body Effects in Core-Level Spectroscopy of Rare-Earth Compounds
(A. Kotani, K. Okada, T. Ikeda and T. Yamazaki)

Core-level photoemission and photoabsorption spectra for various rare-earth compounds, especially for Ce and La compounds, both in metallic and insulating forms are analyzed by using the impurity Anderson model.[1,8,18,20] Important information on $4f$ electron correlation, metallic mixed valency and insulating covalency are obtained from the analysis of $3d$ photoemission spectra.[1,5,8] Spectra of $3p$ core-level are also analyzed.[14] Essential role of the Coulomb interaction between a $4f$ electron and a photo-excited $5d$ electron is shown in the analysis of $2p$ photo-absorption.[5,9,12] Valence photoemission, inverse photoemission and resonant photoemission are also studied.[9,10]

b. Multiplet Structures in Core-Level Spectroscopy
(A. Kotani, K. Okada and H. Ogasawara)

Multiplet structures in photoabsorption and photoemission of $3d$ and $4d$ core electrons in rare earth compounds are studied by incorporating the atomic multiplet coupling described by the Slater integrals and the spin-orbit interaction in the impurity Anderson model. It is shown that the interplay between the atomic multiplet coupling and the solid state hybridization plays an essential role in determining the spectral shape of mixed-valence materials.[2,3,13,22]

c. X-ray Emission Spectra in Insulating Rare-Earth Compounds
(A. Kotani, Y. Kayanuma, S. Tanaka and A. Mori)

X-ray emission spectra corresponding to the $4f \rightarrow 3d$ and $5p \rightarrow 3d$ transitions in insulating Ce and La compounds are calculated by applying the formalism of second order optical process to the impurity Anderson model with a filled valence band. It is shown that the X-ray emission reflects strongly the competition between the dynamical relaxation of

$4f$ electron through the hybridization with the valence band and the lifetime relaxation of the $3d$ core hole.[11,16,18,21] The effect of post collision interaction (changeover from sudden to adiabatic approximation) on X-ray emission spectra as well as on Auger electron spectra is investigated theoretically with simplified models.

d. High-Energy Spectroscopy in High T_c Superconductors
(K. Okada, A. Kotani, H. Katayama-Yoshida, S. Tanaka and Y. Seino)

The filled band Anderson model approach, by which we have already succeeded in describing rare earth compounds, is applied for the analysis of high energy spectroscopy in high T_c superconducting materials, such as $(La_{1-x}Sr_x)_2CuO_4$ and $YBa_2Cu_3O_{7-\delta}$. The model is improved by introducing five filled valence bands to take account of the symmetry of the Cu $3d$ orbitals. From the analysis of the Cu $2p$ photoemission, Cu $3p$ resonant photoemission, Cu L_3 photoabsorption and X-ray emission spectra, strong electron correlation between Cu $3d$ electrons and strongly mixed-valent nature of the ground state are pointed out.[14,15,23] Paying particular attention to the observed polarization dependence of L_3 photoabsorption,[3,4,6] the symmetry of the orbital state of doped holes is discussed in detail.[15,19]

(II) DYNAMICAL PROCESSES IN EXCITED STATES
(Y. Kayanuma)

a. Nonlinear Optical Processes in Condensed Matter

A dynamical theory of coherent nonlinear optical processes is worked out for localized electron-phonon systems. Theoretical predictions for stationary as well as transient responses in the strongly coupled system are presented.[24]

b. Zero-Dimensional Excitons

The quantum size effect of the microcrystals of semiconductor is studied by a model of spherical quantum well. The change of the optical responses is clarified as a function of the ratio of the well radius to the effective Bohr radius of the exciton.[25]

(III) MONTE CARLO STUDY OF SPIN SYSTEMS
(Y. Okabe)

a. Quantum Monte Carlo Simulation

The discovery of the high-T_c superconductors has brought about a renewed interest in two-dimensional quantum spin systems. We systematically study the spin 1/2 quantum XXZ model on the square lattice using the quantum Monte Carlo simulation[26–28] and the exact diagonalization study of the 4×4 system.[29] A special attention is paid to the symmetry breaking in the ground state of the quantum antiferromagnetic spin systems.

b. Ising Spins on Quasicrystals

Using the Monte Carlo simulation, we study the Ising model on quasicrystals. We deal with the two-dimensional Penrose lattice and the three-dimensional icosahedral lattice. The antiferromagnetic spins on the frustrated quasi-lattices are carefully studied.[30–32)]

c. Growth Process of Order Parameter

We study the temporal evolution of the probability distribution function of the order parameter in the ordering process by the Monte Carlo simulation. The dynamical finite-size scaling is shown to hold for the evolution of the probability distribution function. We propose a new method for calculating the effective potential which governs the growth process.[33)]

(IV) ELECTRONIC STRUCTURE OF DEEP IMPURITY STATE IN SEMICONDUCTORS

(H. Katayama-Yoshida)

a. Transition Metal Impurities in II-VI Semiconductors

A unified picture of the electronic structure of Cr impurities in ZnS is presented on the basis of first-principles spin-polarized Green's function calculations. The results obtained on physical properties (donor and acceptor ionization energies, hyperfine coupling constants, g values and Jahn-Teller distortion) are in good agreement with the experimental data, and further clarify the interplay between ionicity and covalency in II-VI compound semiconductors.

b. Mechanism of Hydrogen Passivation in Semiconductors

The electronic structure of hydrogen (H) and boron (B) acceptor complexes in silicon in order to understand the mechanism of hydrogen passivation in silicon. The atomic configuration and electronic structure of H-B complexes are determined using a norm-conserving pseudopotential and supercell method with calculating the Hellmann-Feynman force. Two possible mechanisms for neutralizing the shallow acceptor levels in p-type silicon are considered; (1) H atom is located at the bond center of a Si-B covalent bond and H makes a strong covalent bond with a Si atom, terminating the dangling bond of Si, so that B has three-coordinated covalent bonds with Si atoms, (II) the H atom is located at interstitial antibonding site of a Si-B covalent bond and H becomes H^+ and B becomes B^- due to charge transfer. We find that H is stable at the bond center of a Si-B covalent bond with the large relaxation is included.

(V) MECHANISM OF HIGH-T_c OXIDE SUPERCONDUCTORS

(H. Katayama-Yoshida and Y. Okabe)

a. Isotope Effect in High-T_c Oxide Superconductors

An oxygen isotope effect is observed in Bi-Sr-Ca-Cu-O superconductors when ^{18}O is substituted for ^{16}O. The superconducting transition temperature T_c is lowered by about 0.3-0.4 K. This result suggests a measurable contribution to the superconductivity from phonons. The copper isotope effect is also studied for Y-Ba-Cu-O.

b. NMR Study of ^{17}O of High-T_c Superconductors

Nuclear-spin lattice relaxation rate and Knight shift have been studied by NMR to elucidate the superconducting states and the origin of the pairing mechanism.

Publications

1) *Many-Body Effects in Core-Level Spectroscopy of Rare-Earth compounds*, A. Kotani, T. Jo and J. C. Parlebas, Adv. Phys. **37** (1988) 37.
2) *Effects of Valence Mixing on Multiplet Structure in Core Photoabsorption Spectra for Ce Compounds*, T. Jo and A. Kotani, Phys. Rev. B **38** (1988) 830.
3) *Narrowing Due to Valence Mixing in the 3d Core Level Spectra for Ce Compounds*, T. Jo and A. Kotani, J. Phys. Soc. Jpn. **57** (1988) 2288.
4) *Determination of the Symmetry of the $3d^9\underline{L}$ States by Polarized Cu L_3 XAS Spectra of Single Crystal $YBa_2Cu_3O_{\sim 6.9}$*, A. Bianconi, M. De Santis, A. M. Flank, A. Fontaine, P. Lagarde, A. Marcelli, H. Katayama-Yoshida and A. Kotani, Physica C **153-155** (1988) 1760.
5) *Many-Body Effects in Praseodymium Core-Level Spectroscopy of PrO_2*, A. Bianconi, A. Kotani, K. Okada, R. Giorgi, A. Gargano, A. Marcelli and T. Miyahara, Phys. Rev. B **38** (1988) 3433.
6) *Symmetry of the $3d^9$ Ligand Hole Induced by Doping in $YBa_2Cu_3O_{7-\delta}$*, A. Bianconi, M. De Santis, A. Di Cicco, A. M. Flank, A. Fontaine, P. Lagarde, H. Katayama-Yoshida and A. Kotani, Phys. Rev. B **38** (1988) 7196.
7) *Symmetry of the Hole States in BiCaSrCuO High-T_c Superconductors*, A. Bianconi, P. Castrucci, M. De Santis, A. Di Cicco, A. Fabrizi, A. M. Flank, P. Lagarde, H. Katayama-Yoshida, A. Kotani A. Marcelli, Z. Zhongxian and C. Politis, Modern Phys. Letters B **2** (1988) 1313.
8) *Many Body Effects in Core-Level Spectroscopy of Solids*, A. Kotani, in *Core-Level Spectroscopy in Condensed Systems*, ed. J. Kanamori and A. Kotani (Springer-Verlag, 1988) p. 3 (Proc. 10th Taniguchi Intl. Symp., Kashikojima, 1987).
9) *Theory of High Energy Spectroscopy in CeO_2*, T. Jo and A. Kotani, in *Core-Level Spectroscopy in Condensed Systems*, ed. J. Kanamori and A. Kotani (Springer-Verlag, 1988) p. 34 (Proc. 10th Taniguchi Intl. Symp., Kashikojima 1987).
10) *Resonant Photoemission Spectra of Ce Compounds*, K. Okada and A. Kotani, in *Core-Level Spectroscopy in Condensed Systems*, ed. J. Kanamori and A. Kotani (Springer-Verlag, 1988) p. 64 (Proc. 10th Taniguchi Intl. Symp., Kashikojima, 1987).

11) *Secondary X-Ray Radiation by Core-Level Excitation*, Y. Kayanuma and A. Kotani, in *Core-Level Spectroscopy in Condensed Systems*, ed. J. Kanamori and A. Kotani (Springer-Verlag, 1988) p. 72 (Proc. 10th Taniguchi Intl. Symp., Kashikojima, 1987).

12) *Final State Interaction in L_3 Absorption Spectra of Ce and La Compounds*, A. Kotani, in *Narrow-Band Phenomena*, ed. J. C. Fuggle, G. A. Sawatzky and J. W. Allen (Plenum, 1988) p. 179 (Proc. NATO Workshop on Narrow-Band Phenomena, Staverden, 1987).

13) *Valence Mixing and Multiplet Structure of Core Photoabsorption Spectra in Ce Compounds*, T. Jo and A. Kotani, J. Magn.& Magn. Mater. **76&77** (1988) 361 (Proc. 6th Intl. Conf. on Crystalline Field and Anomalous Mixing Effects in f-Electron Systems, Frankfurt, 1988).

14) *Correlation Satellite in Deep Metal 3p Core X-Ray Photoemission of Tetravalent Oxides MO_2 (M=Ce, Pr, Tb, Hf,) and of LaF_3*, A. Bianconi, T. Miyahara, A. Kotani, Y. Kitajima, T. Yokoyama, H. Kuroda, M. Funabashi and H. Arai, Phys. Rev. B **39** (1989) 3380.

15) *High Energy Spectroscopy in Oxide Superconductors*, K. Okada and A. Kotani, J. Phys. Soc. Jpn. **58** (1989) 1095.

16) *Theory of X-Ray Emission Spectra in La and Ce Compounds*, S. Tanaka, H. Ogasawara, Y. Kayanuma, and A. Kotani, J. Phys. Soc. Jpn. **58** (1989) 1087.

17) *Theory of X-Ray Emission in High-T_c Superconductors*, S. Tanaka, K. Okada, and A. Kotani, J. Phys. Soc. Jpn. **58** (1989) 813.

18) *Core-Level Spectroscopy in Rare Earth Compounds.*, A. Kotani, Solid State Physics **23** (1988) 825 (in Japanese).

19) *Where are the Holes?*, A. Kotani, Parity **3** (1988) 36 (in Japanese).

20) *Optical Properties of Core Electrons*, A. Kotani, in *New Concepts in Solid State Physics* (Baifukan, 1988), p. 103 (in Japanese).

21) *Theory of X-ray Emission spectra in Ce Compounds*, S. Tanaka, Y. Kayanuma and A. Kotani, J. Physique **49** (1988) C8-735.

22) *Multiplet strauctures in 4d-XAS of CeO_2 and $CeRh_3$*, T. Jo and A. Kotani, J.Physique **49** (1988) C8-739.

23) *Theory of Cu 2p-XPS and Resonant XPS in Oxide Superconductors*, K. Okada and A. Kotani, J. Physique **49** (1988) C8-2245.

24) *Ultrafast Relaxation of Localized Excitations in Solids*, Y. Kayanuma, in *Ultrafast Phenomena VI* (Springer, 1988) p. 269 (Proc. 6th Intl. Conf. on Ultrafast Phenomena, Mt. Hiei, 1988) ed. T. Yajima, K. Yoshihara, C.B.Harris and S. Shionoya.

25) *Quantum-Size Effects of Interacting Electrons and Holes in Semiconductor Microcrystals with Spherical Shape*, Y. Kayanuma, Phys. Rev.B **38** (1988) 9797.

26) *Monte Carlo Study of Quantum Spin Systems on the Square Lattice*, Y. Okabe and M. Kikuchi, J. Physique **49** (1988) C8-1393.

27) *Quantum Monte Carlo Simulation of the Spin 1/2 XXZ Model on the Square Lattice*, Y. Okabe and M. Kikuchi, J. Phys. Soc. Jpn. **57** (1988) 4351.

28) *Comment on 'Spin Dynamics in the Square-Lattice Antiferromagnet'*, Y. Okabe, M. Kikuchi and A. D. S. Nagi, Phys. Rev. Lett. **61** (1988) 2971.

29) *Exact Diagonalization Study of the Spin 1/2 XXZ Model on the* 4×4 *Square Lattice*, M. Kikuchi and Y. Okabe, J. Phys. Soc. Jpn. **58** (1989) 679.
30) *Duality in the Ising Model on the Quasicrystals*, Y. Okabe and K. Niizeki, J. Phys. Soc. Jpn. **57** (1988) 1536.
31) *Phase Transition of the Ising Model on the Two-Dimensional Quasicrystals*, Y. Okabe and K. Niizeki, J. Physique **49** (1988) C8-1387.
32) *Statistical Physics of Spin Systems on Quasicrystals*, Y. Okabe, Solid State Physics **24** (1989) 151 (in Japanese).
33) *Growth Process of Order-Parameter Structure — Block-Spin Analysis —*, M. Kikuchi and Y. Okabe, in *Dynamics of Ordering Process in Consensed Matter*, ed. S. Komura and H. Furukawa (Plenum, New York, 1988) p. 57.
34) *Mechanism of Hydrogen Passivation in Silicon*, T. Sasaki and H. Katayama-Yoshida, The Proceedings of 3rd Int. Conference of Shallow Impurities in Semiconductors, Linchoping, Sweden. Inst. Phys. Conf. Sor., No. 95, Chapter 7, p. 395.
35) *Atomic Configuration and Electronic Structure of Anormalous Muon in Silicon*, T. Sasaki and H. Katayama-Yoshida, The Proceedings of 19th Int. Conference on Physics of Semiconductors, Warsow, 1988, ed. W.Zawadzki, p. 1003.
36) *Electronic Structure of Hydrogen and Shallow Acceptor Complexes in Silicon*, T. Sasaki and H. Katayama-Yoshida, The Proceedings of 15th Int. Conference of Defect in Semiconductors, Budapest, Hungary, 1988.
37) *Electronic Structure Calculation and Materials Design System*, H. Katayama-Yoshida and K. Terakura, Solid State Physics, **24** (1989) 277 (in Japanese).
38) *Growth and Characterization of* $YBa_2Cu_3O_{7-x}$ *Single Crystals*, H. Katayama-Yoshida, T. Yonezawa, H. Hirooka, Y. Okabe. T. Takahashi, T. Sasaki, M. Hongoh, K. Yamada, T. Suzuki, S. Hirooka, M. Sato, T. Ciszek and S. K. Deb, Physica C **153-155** (1988) 425.
39) *Photoemission Study of Single Crystalline* $(La_{1-x}Sr_x)_2CuO_4$, T. Takahashi, F. Maeda, H. Katayama-Yoshida, Y. Okabe, T. Suzuki, A. Fujimori, S. Hosoya, S. Shamoto and M. Sato, Phys. Rev. B **37** (1988) 9788.
40) *Oxygen Isotope Effect in the Superconducting Bi-Sr-Ca-Cu-O System*, H. Katayama-Yoshida, T. Hirooka, A. Oyamada, Y. Okabe, T. Takahashi, T. Sasaki, A. Ochiai, T. Suzuki, A. J. Mascarenhas, J. I. Pankove, T. Ciszek and S. K. Deb, Physica C **156** (1988) 481.
41) *Isotope Effect in Oxide High-*T_c *Superconductors*, H.Katayama-Yoshida, Parity **3** (1988) 56 (in Japanese).
42) *Symmetry of the Hole States in Single Crystals of High-*T_c *Superconductors*, A. Bianconi, P. Castrucci, M. De. Santis, A. Di. Cicco, A. M. Flank, P. Lagarde, H. Katayama-Yoshida, A. Marcelli and Z. Zhongxian, International J. of Modern Phys. B **2** (1988) 1151.
43) *Recent Research Related to the Mechanism of High-*T_c *Superconductivity*, H. Katayama-Yoshida, T. Takahashi, H. Matsuyama, Y. Okabe, Y. Kitaoka, K. Ishida, K. Asayama, H. Fujimoto and H. Inokuchi, Proceedings of Adriatico Research Conference on *Towards the Theoretical Understanding of High-*T_c *Superconductors* (World Scientific, 1988) p. 737.

44) *Crystal Growth and Superconducting Phase Formation from Bi-Sr-Ca-Cu-O liquid*, T. F. Ciszek, J. P. Goral, C. D. Evans and H. Katayama-Yoshida, J. Cryst. Growth **91** (1988) 312.

45) *NMR and NQR Studies of* ^{17}O *and* ^{63}Cu *in* CuO_2 *Plane of High-*T_c $YBa_2Cu_3O_{6.65}$ *with* T_c*=61K*, K. Ishida, Y. Kitaoka, K. Asayama, H. Katayama-Yoshida, Y. Okabe and T. Takahashi, J. Phys. Soc. Jpn. **57** (1988) 2897.

46) *Anomalous Nuclear Relaxation and Knight Shift Behavior of* ^{207}Tl *in High-*T_c $Tl_2Ba_2CaCu_2O_{6+x}$, K. Fujiwara, Y. Kitaoka, K. Asayama, H. Katayama-Yoshida, Y. Okabe and T. Takahashi, J.Phys. Soc. Jpn. **57** (1988) 2893.

47) *Superconductivity in Heavy Fermion and High-*T_c *Oxides: Similarity and Dissimilarity*, Y. Kitaoka, K. Ishida, K. Fujiwara, T. Kondo, K. Asayama, H. Katayama-Yoshida, Y. Okabe and T. Takahashi, Proceedings of 6th Int. Conference on Crystal-Field Effect and Heavy Fermion Physics, Frankfurt 1988, J. Magn. Magn. Mat. **76&77** (1988) 527.

48) *Evidence from Angle-resolved Resonant Photoemission for Oxygen-2p Nature of the Fermi-liquid States in* $Bi_2CaSr_2Cu_2O_8$, T. Takahashi, H. Matsuyama, H. Katayama-Yoshida, Y. Okabe, S. Hosoya K. Seki, H. Fujimoto, M. Sato and H. Inokuchi, Nature **334** (1988) 691.

49) *Photoemission Study of Single Crystal* $Bi_2Sr_2CaCu_2O_8$, T. Takahashi, H. Matsuyama, H. Katayama-Yoshida, Y. Okabe, S. Hosoya K. Seki, H. Fujimoto, M. Sato and H. Inokuchi, Proceedings of 1st Int. Symposium on Superconductivity (Nagoya, 1988) (Springer-Verlag) p. 175.

50) *Copper Isotope Effect in Raman Scattering on Superconducting* $YBa_2Cu_3O_{7-x}$, A. Mascarenhas, H. Katayama-Yoshida, J. I. Pankove and S. K. Deb, Phys. Rev. B **39** (1989) 4699.

51) *Photoemission Study of* $Bi_2(Sr, Ca)_3Cu_2O_x$, A. Fujimori, S. Takekawa, E. Takayama-Muromachi, Y. Uchida, A. Ono, T. Takahashi, Y. Okabe and H. Katayama-Yoshida, Phys. Rev. B**39** (1989) 2255,

52) *Experimental Approach to the Mechanisms of High-*T_c *Superconductivity*, H. Katayama-Yoshida, T. Takahashi and Y. Okabe, The Proceedings of the 2nd NEC Symposium (Springer-Verlag ed. H. Kamimura and A. Oshiyama) p. 186.

53) *NMR in High-*T_c *Oxide Superconductors*, Y. Kitaoka, K. Ishida, K. Fujiwara, Y. Kohori, K. Asayama, H. Katayama-Yoshida, Y. Okabe and T. Takahashi. The Proceedings of 2nd NEC Symposium (Springer-Verlag ed. H.Kamimura and A.Oshiyama), p. 148.

Master Thesis (March 1989)

Ml) Theory of Photoemission Spectra in Rare Earth Oxides, Tatsuroh Ikeda.